Ab-initio pairing for HFB calculations of (up to heavy) nuclei

T. Duguet

Physics Division, Argonne National Laboratory

Nuclei at the Limits, Argonne, 26-30 july 2004

Structure effects related to pairing

I. Individual excitation spectra:

*Gap for even-even nuclei $\Rightarrow$ a (quite) direct measure of the gap

II. Collective excitations

*Rotational: $\nearrow \mathcal{J}^{(2)} = -\frac{\partial^2 \mathcal{E}^\omega}{\partial^2 \omega}$ with ω

*Vibrational states: low-lying states $\rightarrow$ especially in exotic nuclei

*Shape isomers: from intruders

$\Rightarrow$ more indirect measure but sensitive to the spatial structure of the force

III. Width of deep-hole states

IV. Pair transfer

V. Odd-even mass staggering (OES)

VI. Glitches in the inner crust of neutron stars

VII. Cooling of neutron stars: emission processes and heat diffusion

Main ingredients for pairing

I. The global amount of pairing (in the ground-state as a start) depends on:

*the number N of particles outside a closed-shell

*the density of s.p. states around the Fermi surface $\Leftarrow N$, $m^\star$, level of approx

*the proximity of the s.p. continuum

II. Pairing properties and their trends (toward drip-lines for instance) depend on:

*the characteristics of the (effective? and phenomenological?) pairing force used:

$\longrightarrow$ isoscalar and isovector density-dependence

$\longrightarrow$ range?

*the level of approximation one is working at:

$\longrightarrow$ mean-field = static pairing

$\longrightarrow$ beyond = dynamical pairing

Effective Forces for Mean-Field Calculations of finite nuclei

I. Mean-field = particle-hole channel $\Longrightarrow$ Usually Skyrme or Gogny = “Mimic” a G-matrix

II. Pairing = particle-particle channel ($^1S_0$ channel for now $\Longrightarrow$ n-n and p-p)

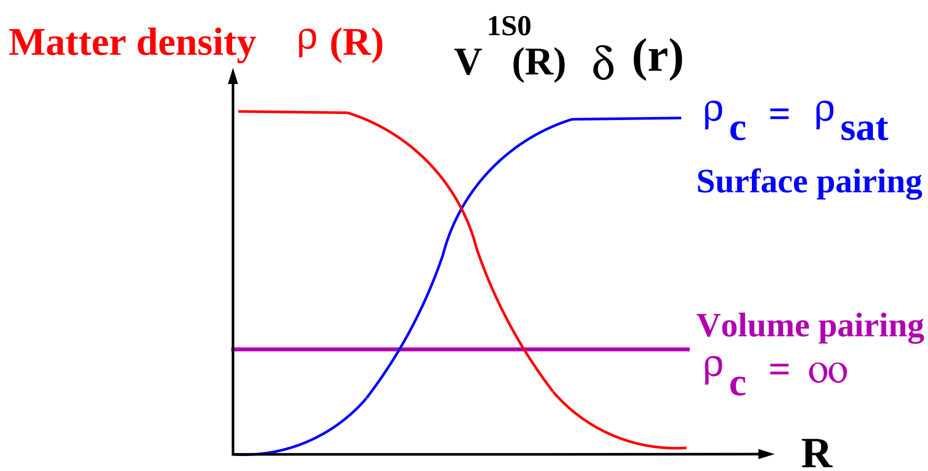
So far, only phenomenological interactions have been used in finite nuclei

- $V_\tau(\vec{r}_1,\vec{r}_2) = \sum_{i=1}^{2} \lambda_\tau^i \, e^{-|\vec{r}_1-\vec{r}_2|^2/\alpha_i^2}$ $\Longrightarrow$ Finite-range/Density-independent
- $V_\tau^{^1S_0}(\vec{r}_1,\vec{r}_2) = \lambda_\tau \left[1 - \rho(\frac{\vec{r}_1+\vec{r}_2}{2})/\rho_c\right] \delta(\vec{r}_1-\vec{r}_2)$ $\Longrightarrow$ Zero-range/Surface-peaked

BCS gap equation:

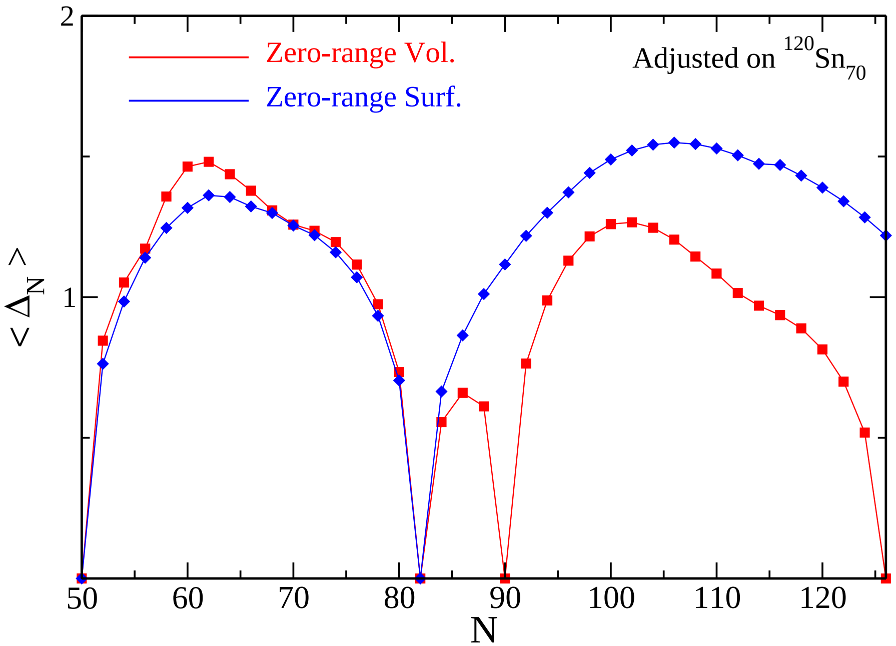
$$\Delta_i = \sum_j \langle i\,\bar{i}\,|\,V\,|\,j\,\bar{j}\rangle \frac{\Delta_j}{2E_j}$$

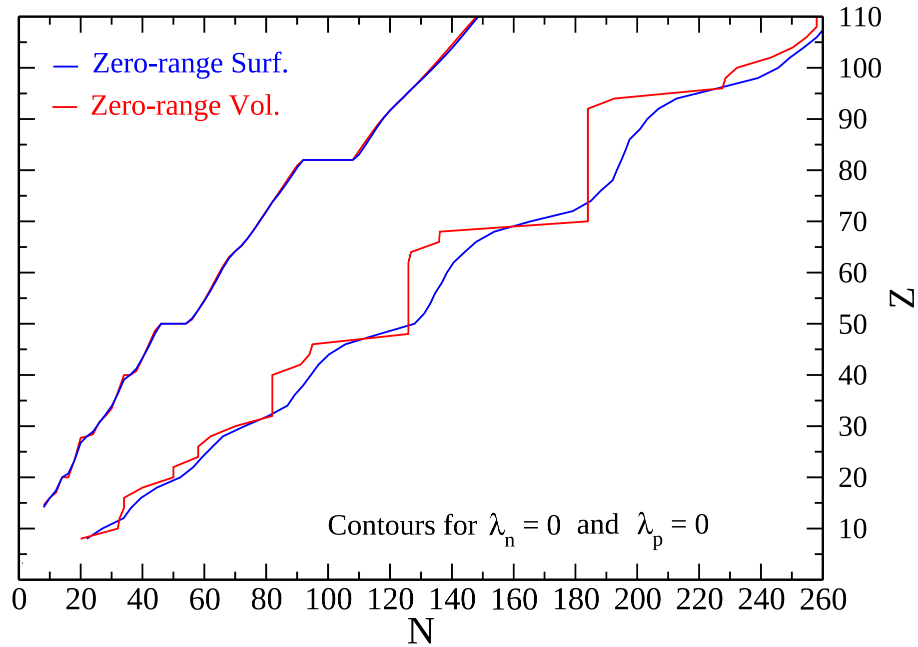
=> **The zero−range force requires a cut−off in the sum over j**



III. Spherical HFB calculations: Sn isotopes (SLy4 in the p-h channel)

K. Bennaceur *et al.* (2003)





$\longrightarrow$ differences are strongly enhanced in exotic nuclei

$\longrightarrow$ **Isovector dependence is very different**

$\longrightarrow$ **The neutron drip-line can be shifted by 20 mass units!**

Study

I. Puzzles T. Duguet, PRC (2004)

*Existing forces are succesfull over the known mass table

*Limited predictive power for unknown regions

Ab-initio work = connection to the bare NN force is needed

II. Technical issues

*Simple forms required to perform extensive HFB calculations of finite nuclei

*Even more critical when going beyond the mean-field as we do now

III. By-product: we can understand

*Link with usual DDDI ⇒ isovector density-dependence

*Comparing finite vs zero range forces (regularization procedure)

*Contribution of the bare force to pairing in finite nuclei

*what is needed beyond? (QRPA, GCM, Projection, polarization effects)

Link with the bare force: meaningful mean-field picture

From **many-body perturbation theory** written in terms of the bare nucleon-nucleon force:

Green-function's formalism $\Rightarrow$ non-time-ordered diagrams: Galitskii, Migdal, Gorkov...

Goldstone formalism $\Rightarrow$ time-ordered diagrams: Goldstone, Brueckner, Bogolyubov, Mehta...

$\Longrightarrow$ Meaningful **mean-field** picture = lowest-order in terms of **IRREDUCIBLE vertices**

Particle-hole:

In-medium two-body matrix (G or T)

$\longrightarrow$ phenom. Skyrme, Gogny, ... forces

Particle-particle:

Bare interaction (unlike condensed matter)

$\longrightarrow$ phenom. Gogny, DDDI, ... forces

usually in the ${}^1S_0$ channel for finite nuclei

Bare NN force in the $^1S_0$ channel

I. Realistic NN forces in their full glory are too involved

II. Impossible to use in systematic calculations of heavy nuclei

III. A solution

$$\langle \vec{k}_1 \vec{k}_2 \,|\, V^{^1S_0} \,|\, \vec{k}_3 \vec{k}_4 \rangle \approx \lambda \; v(k) \; v(k') \; (2\pi)^3 \, \delta(\vec{P} - \vec{P}\,') \qquad \text{with} \qquad v(k) = e^{-\alpha^2 k^2}$$

$\Longrightarrow$ Very well justified at low energy (virtual di-neutron in the vacuum)

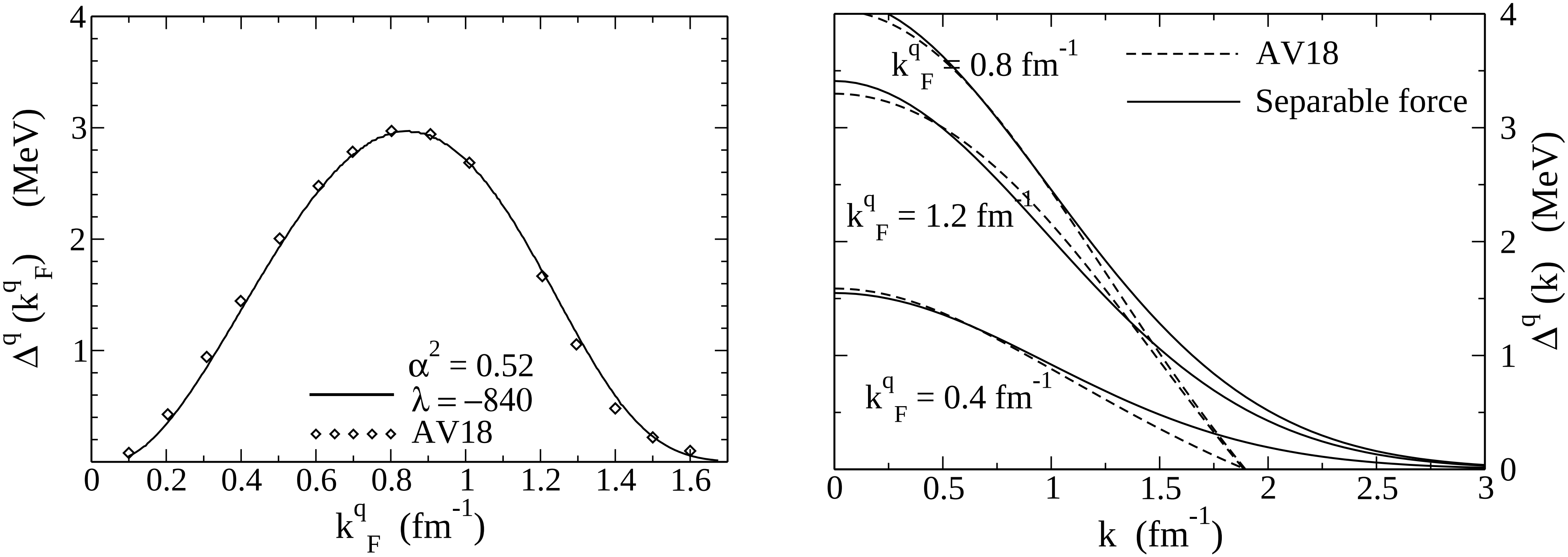
IV. Adjustment

*Phase shifts $\delta^{^1S_0}(k)$ from NN scattering

*Pairing gap from realistic NN interaction in infinite matter

$\Longrightarrow$ We use AV18 NN interaction, R. B. Wiringa *et al.* (1995)

III. Results in infinite matter (no self-energy at this stage: $\epsilon(k) = k^2/2m$)



*The separable force is able to reproduce fine pairing properties:

$\Delta^q(k_F)$ up to the gap closure AND $\Delta^q(k)$ $\forall\, k$

*The Gogny force is close to $V^{^1S_0}$

IV. Self-consistent HFB calculations of finite nuclei in coordinate space: $V^{^1S_0}$ is still untractable

V. Link to density-dependent zero-range interactions: not obvious

VI. Reformulation of the pairing problem in terms of an effective force

$$\Delta^q_{i\bar{i}} = -\sum_{j>0} \langle i\,\bar{i}\,|\,V^{^1S_0}\,|\,j\,\bar{j}\,\rangle\, u_j\, v_j \iff \Delta^q_{i\bar{i}} = -\sum_{j>0} \langle i\,\bar{i}\,|\,\mathcal{D}^{^1S_0}[k^q_F](P,0)\,|\,j\,\bar{j}\,\rangle\, 2\,v_j^2\;\, u_j\, v_j$$

where $\mathcal{D}^{^1S_0}$ sums scattering p-p and h-h ladders in the **superfluid** system:

$$\langle\, i\, j\,|\,\mathcal{D}^{^1S_0}[k^q_F](P,s)\,|\,k\,l\,\rangle = \langle\, i\, j\,|\,V^{^1S_0}\,|\,k\,l\,\rangle - \sum_{mn} \langle\, i\, j\,|\,\mathcal{D}^{^1S_0}[k^q_F](P,s)\,|\,m\,n\,\rangle\, \frac{1 - v_m^2 - v_n^2}{E_m + E_n + 2\,s}\, \langle\, m\,n\,|\,V^{^1S_0}\,|\,k\,l\,\rangle$$

VII. Effective pairing interaction:

*takes care of high-E virtual excitations in the gap equation

*introduce a natural **cut-off** through $2v_j^2$ measured / ϵ_F

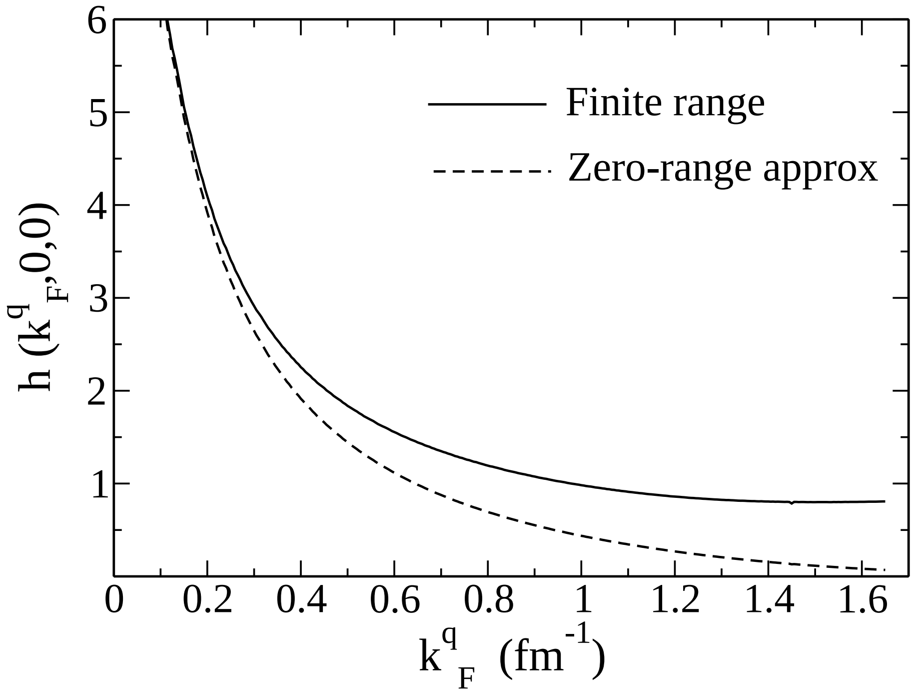
*density dependent: k^q_F

$\Rightarrow$ Appropriate scheme to study **range vs density-dependence**

The effective interaction in infinite matter

I. Form $\langle \vec{k}\,|\,\mathcal{D}^{^1S_0}(k_F^q, P, 0)\,|\,\vec{k}\,'\rangle = \lambda\ v(k)\ h(k_F^q, P, 0)\ v(k')$

II. Density dependence: $h(k_F^q, 0, 0)$



*Enhanced at low-density $\Longrightarrow$ surface enhancement through LDA

*No finite size effect so far

*Zero-range approximation: stronger "surface versus volume" enhancement

The effective interaction in coordinate space

*The force is finite-ranged, non-local, density-dependent

$$\langle \vec{r}_1 \vec{r}_2 \,|\, \mathcal{D}_q^{^1S_0}[\rho_q(\vec{r})](0) \,|\, \vec{r}_3 \vec{r}_4 \rangle = \frac{\lambda}{(2\pi)^6 \alpha^{12}} \int d\vec{r}\; C\left(\rho_q(\vec{r})\right)\; e^{-\sum_{i=1}^{4} |\vec{r}-\vec{r}_i|^2/2\alpha^2}$$

with $C\left(\rho_q(\vec{r})\right) \equiv h(k_F^q(\vec{r}), 0, 0)$ from LDA

II. Calculation of Δ_{ik} requires $(V_q^{eff})_{ikjl}\ \forall\ (jl)$ $\Leftrightarrow$ set of quadrupole integrals, BUT

$$(V_q^{eff})_{ikjl} = \lambda\,(v_j^2 + v_l^2) \sum_{ss'} \int d\vec{r}\; C\left[\rho_q(\vec{r})\right]\; \tilde{\varphi}_{n_i qs}(\vec{r})\, \tilde{\varphi}_{n_k qs'}(\vec{r}) \left\{ \tilde{\varphi}_{n_j qs}(\vec{r})\, \tilde{\varphi}_{n_l qs'}(\vec{r}) - \tilde{\varphi}_{n_j qs'}(\vec{r})\, \tilde{\varphi}_{n_l qs}(\vec{r}) \right\}$$

with $\tilde{\varphi}_{nqs}(\vec{r}) = \frac{1}{(\sqrt{2\pi}\,\alpha)^3} \int d\vec{r}\,'\, e^{-|\vec{r}-\vec{r}\,'|^2/2\alpha^2}\, \varphi_{nqs}(\vec{r}\,')$

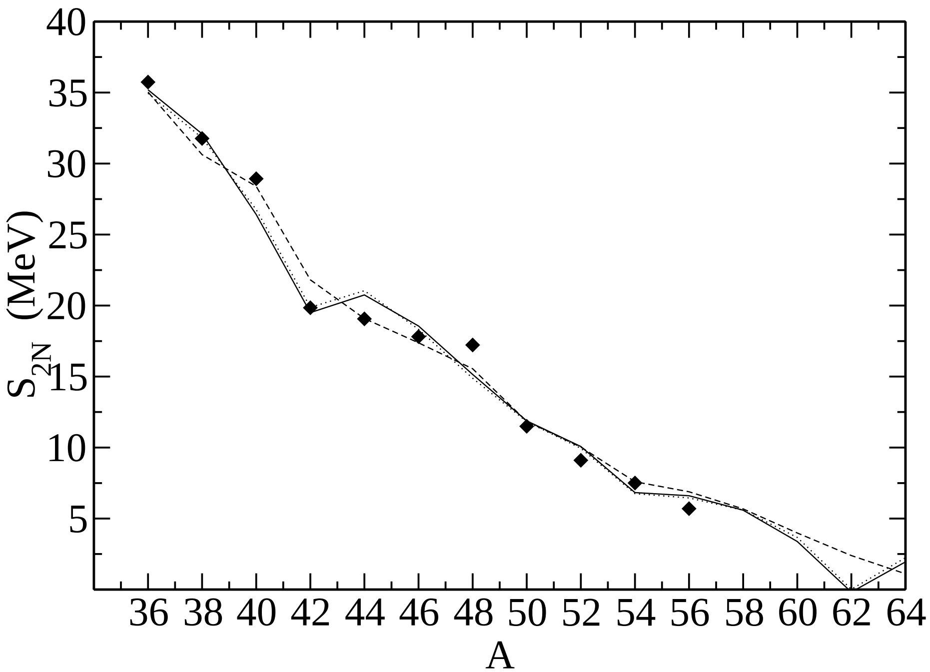
*Computational cost $\approx$ zero-range force $\Rightarrow$ 3D HFB calculations in coordinate space tractable

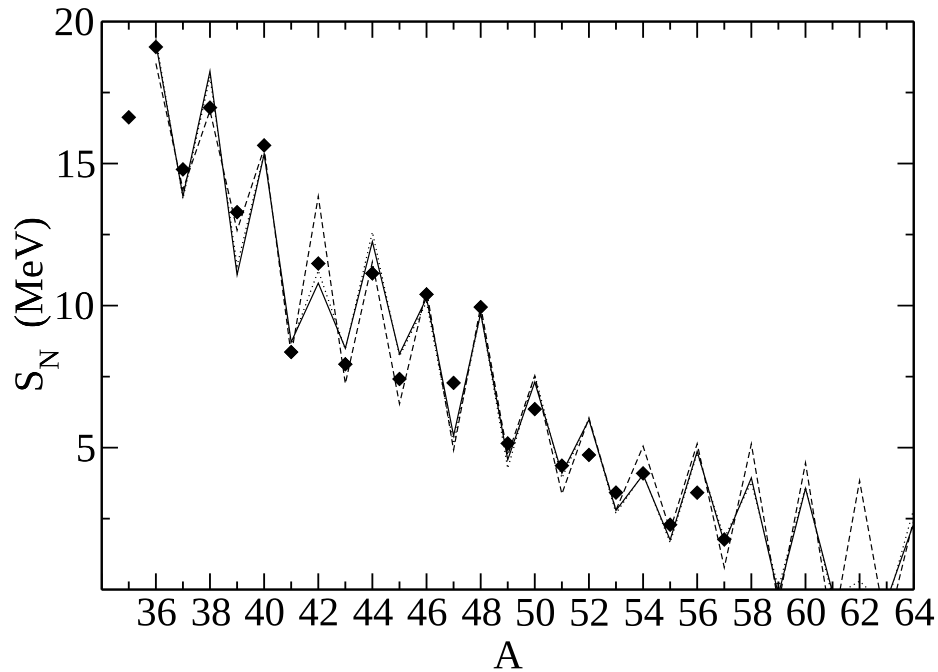
*Requires only trivial modifications of existing codes

Ca isotopes - pairing toward the drip-lines

Self-consistent 3D HFB calculations - SLy4 Skyrme force in the p-h channel

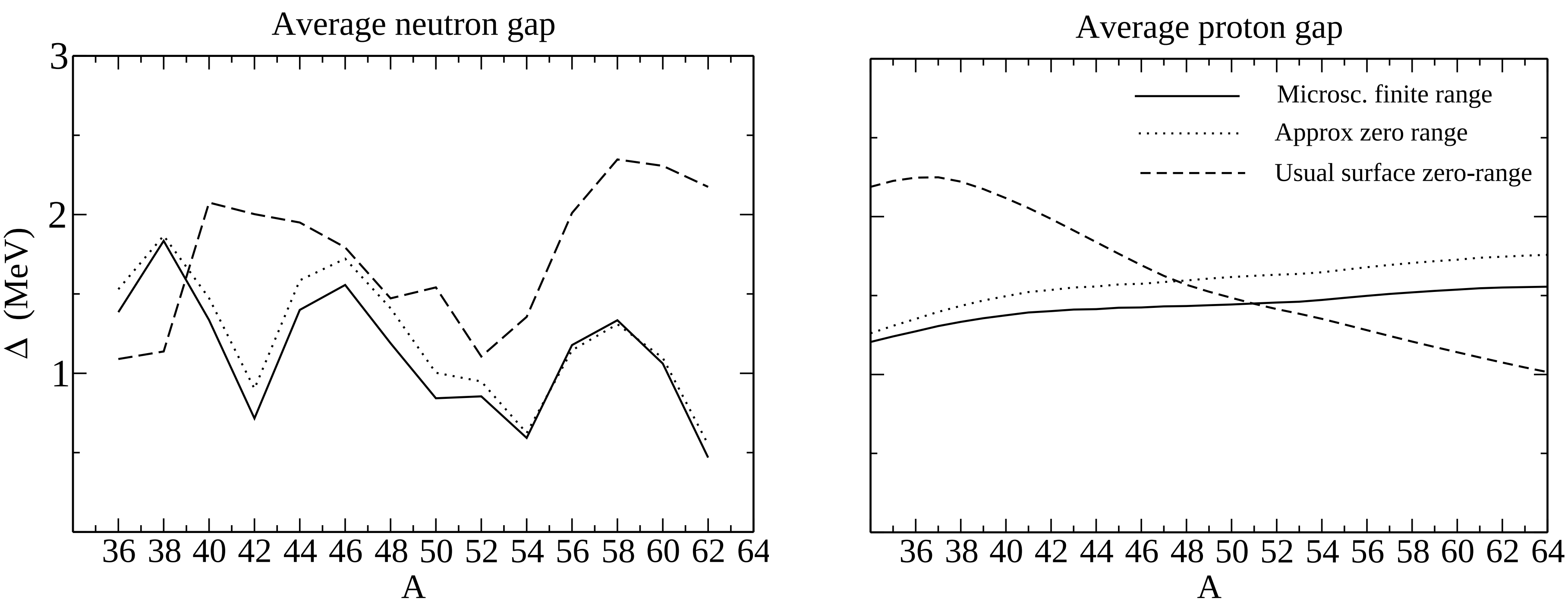
*S_{2N} and S_N including Time-Reversal-Symmetry-Breaking in odd nuclei





One example: Ca isotopes - pairing toward the drip-lines

Self-consistent 3D HFB calculations - SLy4 Skyrme force in the p-h channel



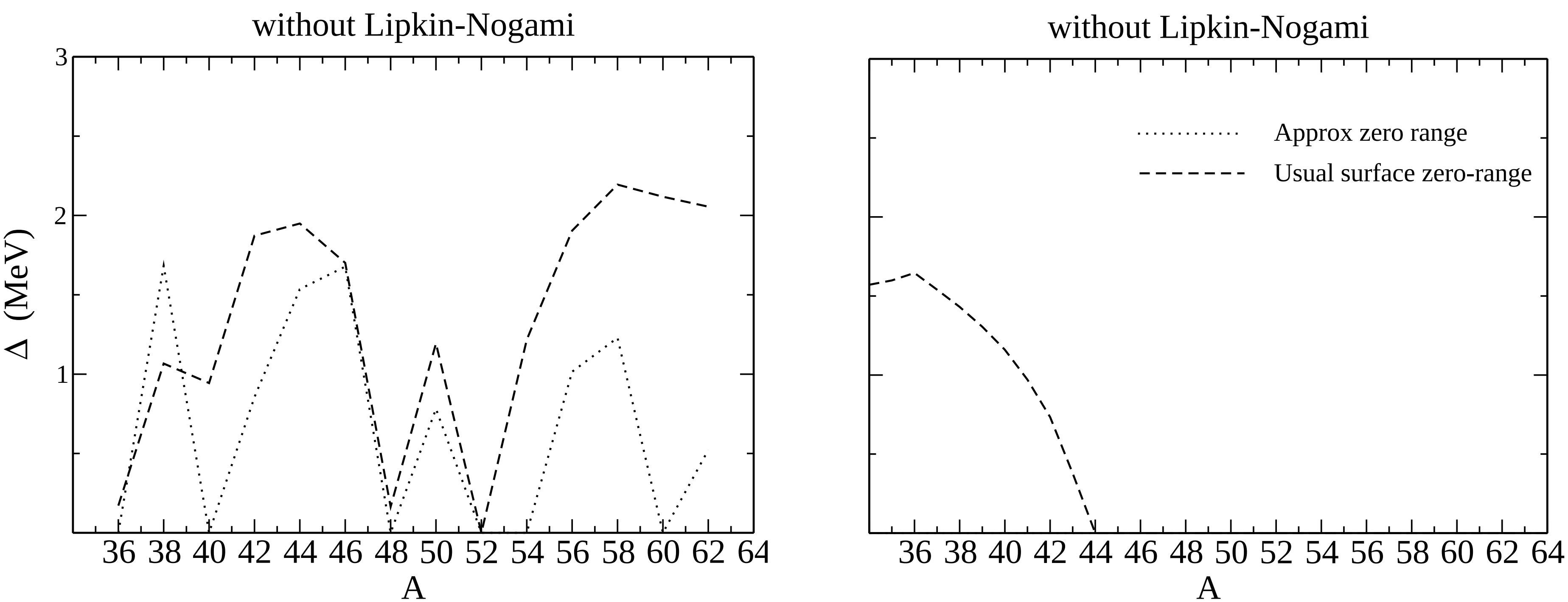
*Average gap: $\bar{\Delta}^q = \sum_n u_n v_n \Delta^q_{n\bar{n}} / \sum_n u_n v_n$ in the canonical basis

*Usual surface-delta interactions: $\lambda_\tau \left(1 - \rho(\vec{R})/\rho_c\right) \delta(\vec{r})$ has a very different isovector trends

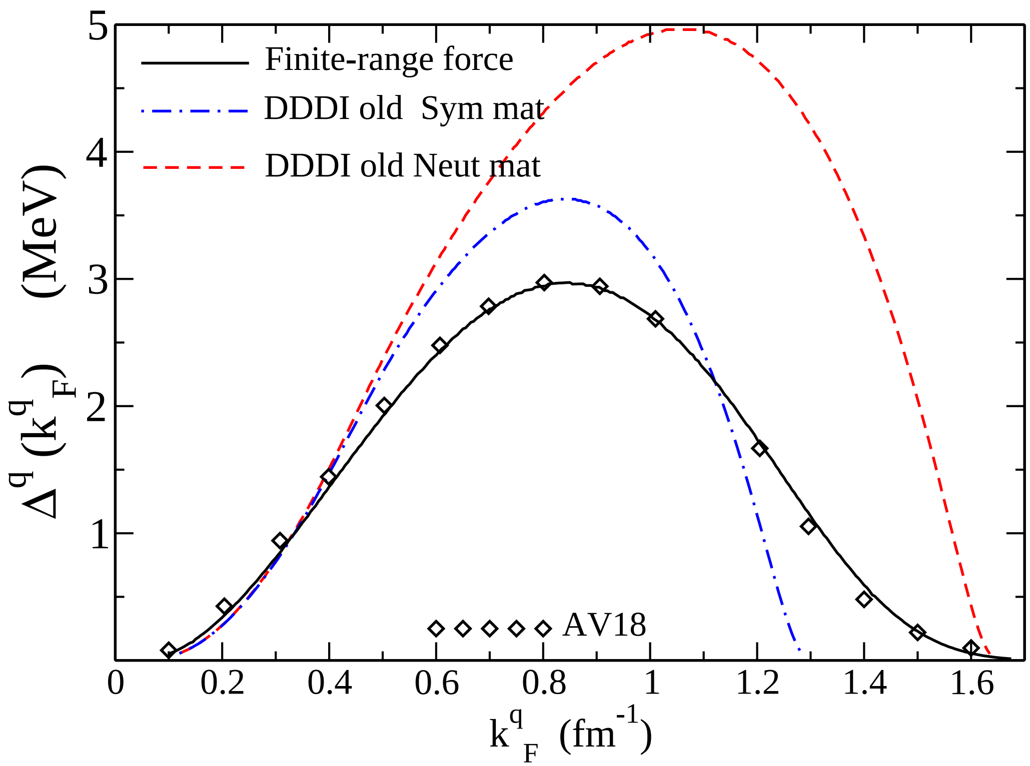
*We are looking at the contribution of the bare NN force to pairing in finite systems

Ca isotopes - pairing toward the drip-lines

*Average gaps without Lipkin-Nogami



Isovector trend in nuclear matter



*Zero-range forces depending on the total density $\rho(\vec{R})$ have a wrong isovector nature

*Overestimate (underestimate) the neutron (proton) pairing at the neutron (proton) drip-line

Perspectives

I. Extensive study through HFB calculations (K. Bennaceur, P. Bonche and G. Bertsch)

*Softness of the interaction: much better than Gogny = tractable in coordinate space

$\longrightarrow$ can be used for microscopic mass tables

*Odd-even mass differences, moment of inertia

$\longrightarrow$ Systematic study of bare force's contribution to pairing in finite nuclei

*Systematic study of the role of the finite-range in both ground-states and excited states

II. Some questions for the (near) future

*Beyond mean-field: Projection + GCM methods (M. Bender, P. Bonche and P.-H. Heenen)

*Effect of the three-body force in the pairing

*Need for Coulomb to describe proton-proton pairing